Stabilised Wilson Fermions for the Intensity Frontier

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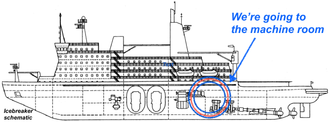

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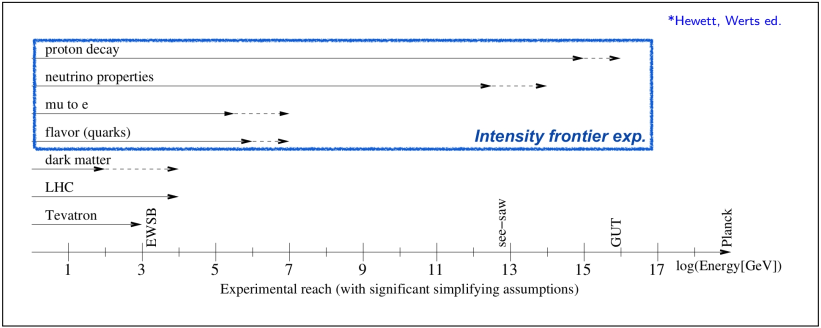
The Intensity frontier



- Fundamental physics with intense sources and ultra-sensitive detectors.
- Precision studies of the SM and beyond.
- Greatest possible beam intensities of neutrinos, electrons, muons, photons and hadrons.
- Experimental programs FRIB, Muon G-2, Project X, EIC (@BNL) ...

*Hewett, Werts ed., https://www.slac.stanford.edu/econf/C1307292/docs/Intensity-2.pdf

At the intensity frontier "lattice QCD plays a crucial role"

*Hewett, Werts ed., https://www.slac.stanford.edu/econf/C1307292/docs/Intensity-2.pdf

Example calculations are

- $(g-2)_\mu$: Resolve tension with SM, new physics
- *Flavour physics:* Rare decays (K, D, B), *cp* violation
- *Multi-nucleons:* Nuclear physics
- *Hadron structure:* Proton spin, radius, magnetic moment, ...
- *Parton distribution functions:* Proton structure

A technical frontier for lattice QCD

Addressing their systematics we face different challenges:

- $(g-2)_\mu \rightsquigarrow$ fine, light and large lattices.
- *Flavour physics* $\rightsquigarrow$ very fine lattices.
- *Multi-nucleons* $\rightsquigarrow$ large and coarse lattices.
- *Hadron structure* $\rightsquigarrow$ low Q^2, i.e. large, coarse, light lattices.
- *PDFs* $\rightsquigarrow$ large Q^2, i.e. fine and light lattices.

∘ A common requirement are large lattice volumes.

∘ **But**, as $m_\pi \downarrow$ and/or $V \uparrow$ the spectral gap spec$(D) \downarrow$
$\rightarrow$ Algorithmic instabilities hamper the generation of configurations and can affect observables.

∘ Here we aim to provide some remedies and tools to ameliorate and overcome these problems - with a focus on Wilson-Clover fermions.

Remedies and tools

An often used treatment to stabilise calculations is **smearing**.
- Gauge fields are smoothed in an iterative procedure.
- Degree of smoothing is controlled by smearing parameters.

Here we present extra/alternative tools:

Exponentiation of the usual Clover term.
- Reduces fluctuations induced by the Clover.

Implementation of the Stochastic Molecular Dynamics algo.
- Increases stability in the MD evolution.

Use of V-independent norm and quadruple precision numbers.
- Guarantee of required numerical precision.

Stabilised Wilson fermions are the combination of the last three.

Disclaimer: Some components not new, references given.

$\mathcal{O}(a)$-improvement revisited

- The $\mathcal{O}(a)$-improved Wilson Dirac operator is:

$$D = \frac{1}{2}\Big[\gamma_\mu\Big(\nabla^*_\mu + \nabla_\mu - a\nabla^*_\mu\nabla_\mu\Big)\Big] + c_{SW}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} + m_0$$

- Classifying the lattice points as even/odd one may write

$$D = \begin{pmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{pmatrix}$$

with diagonal part

$$D_{ee} + D_{oo} = 4 + m_0 + c_{SW}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}$$

- E/O-preconditioned form:

$$\hat{D} = D_{ee} - D_{eo}(D_{oo})^{-1}D_{oe}$$

$\mathcal{O}(a)$-improvement revisited: Focus on the Clover

∘ At tree-level $c_{SW} = 1$ and grows monotonically with g_0^2.

$\rightsquigarrow$ $c_{SW} \sim 2$ on coarse lattices.

∘ Pauli term can be fairly large, particularly on coarse lattices, saturating the bound:

$$\left\| \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \right\|_2 \leq 3$$

∘ Positive and negative EV of the Pauli term are equally distributed:

→ D_{oo} is not protected from arbitrarily small EV.

→ Especially so for small masses and rough gauge fields.

→ E/O-preconditioning can fail.

$\rightsquigarrow$ Probability to do so grows with larger lattice volumes.

→ Irrespective of E/O-prec. these fluctuations can spoil the calculation.

$\rightsquigarrow$ **(Coarse, very) large lattice volumes or masterfields not feasible.**

Exponentiated Clover

$\mathcal{O}(a)$-improvement revisited: Exponentiating the Clover

- Alternative definition for the $\mathcal{O}(a)$-improved Wilson Dirac operator:

$$D_{ee} + D_{oo} = (4 + m_0) \exp\left[\frac{c_{SW}}{4 + m_0} \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \right]$$

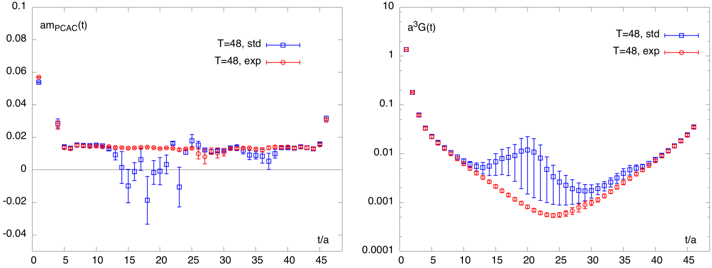
- Definition coincides with previous definition at leading order in a.
- Diagonal part of the Dirac operator is positive definite and safely invertible.
- E/O-preconditioning becomes unproblematic.
- Also, $\det D = \det \hat{D}$ up to a field-independent proportionality constant.

Exponentiated Clover: Quenched theory

◦ Initial tests in quenched theory (Wilson gauge):

→ Non-perturbatively tuned c_{SW} in the massless SF scheme.

→ Pion correlators at $\beta = 6.0$, κ tuned to match Clover and eClover, configurations are identical.



◦ Initial tests show promise:

→ Some indications that fluctuations indeed are reduced.

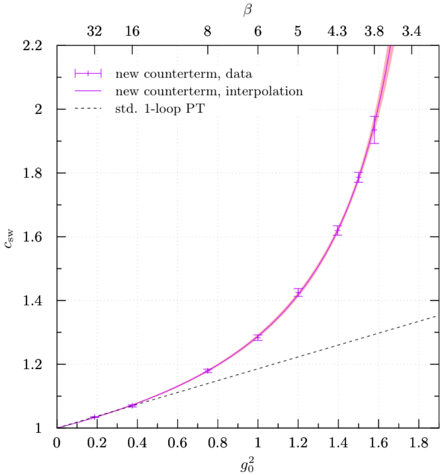
→ **Need tests and verification in full QCD.**

Exponentiated Clover: Full QCD, tuning c_{SW} in the SF

- To test viability and features in full QCD we run in the following:

$\rightarrow$ $n_f = 2 + 1$ QCD with the Lüscher-Weisz gauge action.

$\rightarrow$ Non-perturbatively tune c_{SW} in the massless SF scheme.



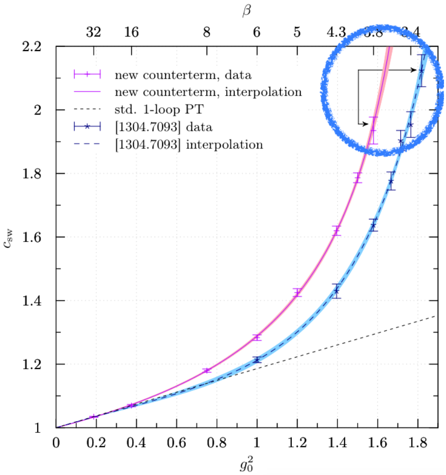
- eClover:

$$M_0 \exp\left[\frac{c_{SW}}{M_0}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\right]$$

$\rightarrow$ These runs use the HMC.

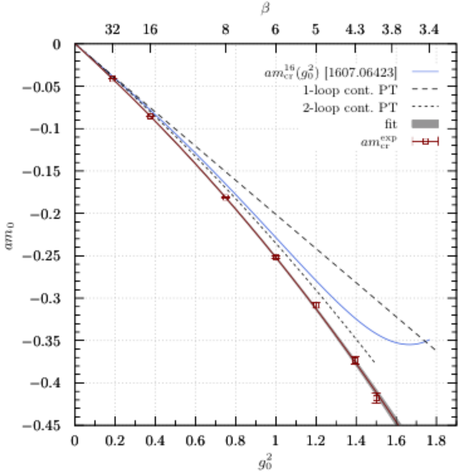
$\rightarrow$ Stable inversions of D_{oo} (1M traj., $\tau = 2$).

Exponentiated Clover: c_{SW} comparison



- ◦ Arrows indicate equal lattice spacing $a[\mathrm{fm}] \simeq 0.095$
- $\rightarrow$ For equal lattice spacing $c_{SW}^{\mathrm{eClov}} < c_{SW}^{\mathrm{Clov}}$.

Exponentiated Clover: Critical mass

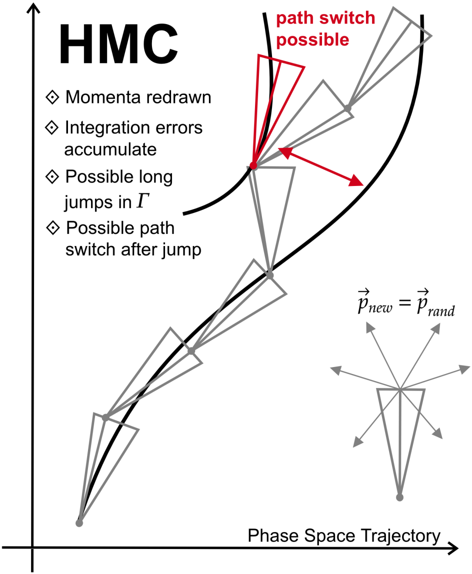


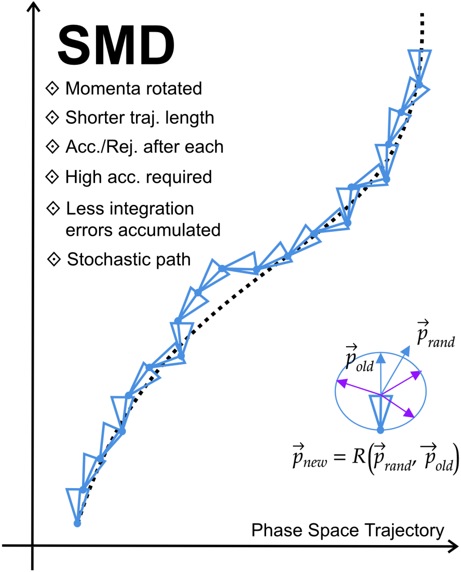
◦ Critical mass:

$$am_{\text{crit}} = \frac{1}{2\kappa_{\text{crit}}} - 4$$

→ We observe a monotonic dependence on g_0^2 with the eClover.

Stochastic Molecular Dynamics





Generally: More spikes in ΔH means longer autocorrelation times.

Stochastic Molecular Dynamics (SMD) algorithm

A. M. Horowitz '85, '87, '91; K. Jansen, C. Liu hep-lat/9506020

◦ Basic components: gauge links $U(x,\mu)$, momentum $\pi(x,\mu)$, pseudo-fermion $\phi(x)$ and action $S_{\text{pf}} = \phi\big(D^\dagger D\big)^{-1}\phi$.

Update cycle

- Refresh $\pi(x,\mu)$ and $\phi(x)$ by a random field rotation

$$\pi \to c_1\pi + c_2 v \quad , \qquad \phi \to c_1\phi + c_2 D^\dagger\eta$$

  $\rightarrow$ v and η random normal distributed
  $\rightarrow$ $c_1^2 + c_2^2 = 1$
  $\rightarrow$ $c_1 = e^{-\epsilon\gamma}$, where ϵ is the MD integration time and γ is a friction parameter

- MD evolution (short)
- Accept/Reject-step (makes the algorithm exact)
- Repeat ⥁

Notes

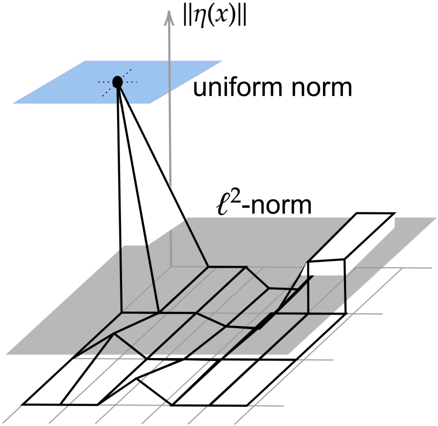
- At fixed ϵ and large γ the SMD coincides with the HMC.
- For small ϵ the SMD can be shown to be ergodic* and to converge to a unique stationary state simulating the canonical distribution.
- When configurations are rejected the momentum is reversed and the trajectory tends to backtrack.
  $\rightarrow$ Rejections should ideally occur only at large distances in τ.
- $\Delta H \propto \sqrt{V}$ implies integration has to be made more precise with $V \uparrow$
  $\rightarrow$ Use high order integration rules.
- SMD has shorter autocorrelation times**. This (largely) compensates the longer time per MDU compared to the HMC.

> - The SMD gives a reduction of unbounded energy violations $|\Delta H| \gg 1$.

*M. Lüscher '17; **M. Lüscher [1707.09758]

Uniform norm, quadruple precision

Further algorithmic improvements



∘ Solver stopping criterion:
Convergence when $\tilde{\psi}$ satisfies

$$\|\eta - D\tilde{\psi}\|_2 \leq w\|\eta\|_2$$

with: $\|\eta\|_2 \propto V$

→ Possibly local fluct. missed
→ But forces derived locally.
→ Uniform norm:

$$\|\eta\|_\infty = \sup_x \|\eta(x)\|_2$$

→ Insurance also for current V.

∘ Accept/Reject: $$\Delta H \propto \epsilon^p \sqrt{V}$$

→ Summing over all lattice points can cause accumulation errors
→ Use quadruple precision in global sums.

Running $n_f = 2+1$ full QCD

∘ In the following we perform: In situ calculations using all stabilising measures and the non-perturbatively tuned c_{SW}.

∘ Chiral trajectory is set via:

$$\phi_4 = 8t_0\left(\frac{1}{2}m_\pi^2 + m_K^2\right) = 1.115 = \text{const.} \propto \mathrm{Tr}[M_q]$$

a[fm]	$L^3 \times T$	m_π[MeV]	m_K[MeV]	$m_\pi L$	BC	status
0.095	$32^3 \times 96$	410	410	6.3	P	done
	$32^3 \times 96$	294	458	4.5	P	done
	$32^3 \times 96$	220	478	3.4	P	done
	$64^3 \times 144$	135	494	4.2	P	planned
0.064	$48^3 \times 96$	410	410	6.4	P	running
0.055	$48^3 \times 96$	410	410	5.5	O	running

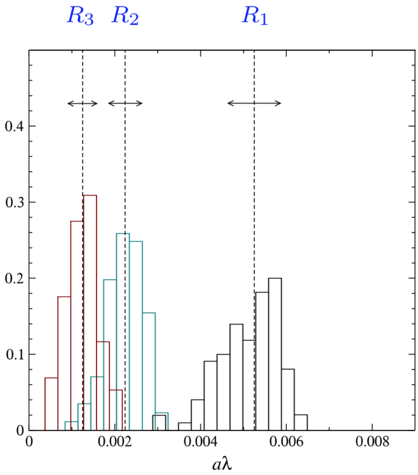
Running $n_f = 2 + 1$ full QCD

- Parameters at $a[\mathrm{fm}] = 0.095$ ($\beta = 3.8$):
  $\gamma = 0.3$, $\epsilon = 0.31$, 2 levels of OMF-4, $N_{pf} \leq 8$, $deg(R) \leq 10$

Label	m_π[MeV]	P_{acc}	$P(\lvert\Delta H\rvert \geq 2)$
R1	410	97.5%	0.15%
R2	294	98.6%	0.15%
R3	220	98.2%	0.05%

- The runs show no issues with stability (also $\beta = 4.0,\ 4.1$).
- Physical m_π seems possible at coarse lattice spacing.
- Lowest eigenvalue of $\sqrt{D^\dagger D}$ measured with less than 0.5% uncertainty.
- Even coarser lattice spacings, $a[\mathrm{fm}] > 0.095$, seem possible.

Spectral gap of the Dirac operator



∘ Smallest eigenvalue behaves as:

$\rightarrow$ $a\lambda = \min\left[\mathrm{spec}\left(D^\dagger D\right)^{\frac{1}{2}}\right]$
$a\lambda[\mathrm{MeV}] \in [0.001, 2]$

$\rightarrow$ Median $\mu \propto Zm_q$

$\rightarrow$ Width $\sigma \downarrow$ for $m_\pi \downarrow$
$\rightsquigarrow$ similar to $n_f = 2^*$

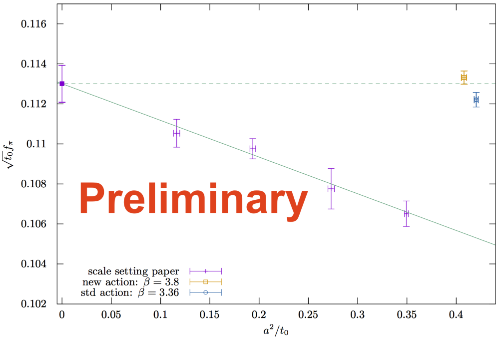
$\rightarrow$ Empirically: $\sigma \simeq a/\sqrt{V}^*$

*L. Del Debbio et al. hep-lat/0701009

∘ $R1, R2, R3$ have about equal computational cost here.
$\rightarrow$ Cost of bigger κ_l is largely compensated by the smaller κ_s.

Towards quantifying cutoff effects

- Scaling tests are still ongoing, all results are preliminary.
- Here: Indications and exploratory studies of cutoff effects.



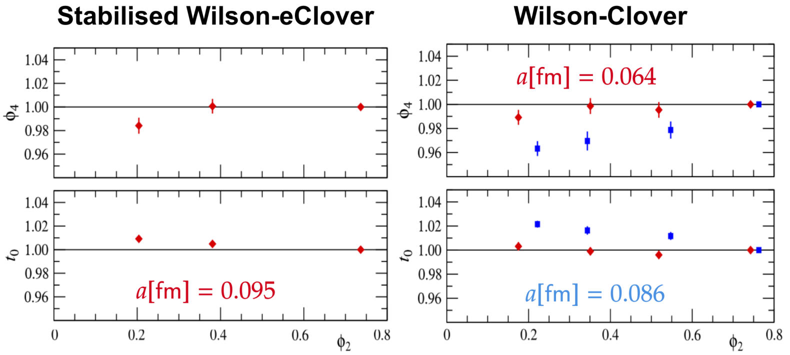
- Comparison to symmetric point data from M. Bruno et al. [1608.08900], where Z_A is from the chirally rotated SF M. Dalla Brida et al. [1905.05147].
- Our points (traditional=blue, stabilised=orange) use Z_A determined via fermion flow M. Lüscher [1302.5246].

Towards quantifying cutoff effects

◦ Note: A fixed bare quark mass trajectory shows deviations of $\mathcal{O}(am)$ for a given observable. M. Bruno et al. [1608.08900]

◦ Opportunity to test and compare for:

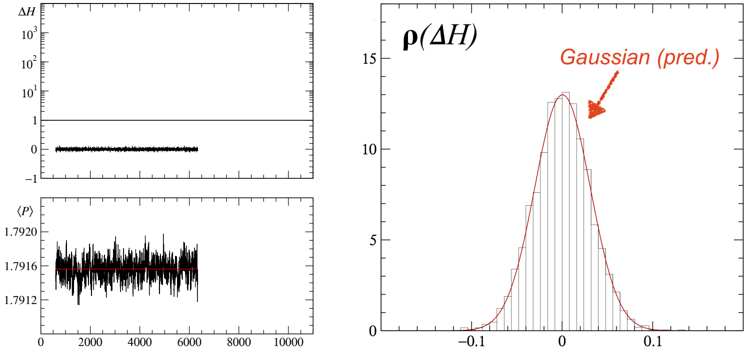
$$\phi_4 = 8t_0\left(\frac{1}{2}m_\pi^2 + m_K^2\right) \quad \text{and} \quad \phi_2 = 8t_0 m_\pi^2$$



CLS runs: H101,H102,C101 (blue), N202,N203,N200,D200 (red)

Runs at finer lattice spacing, $a[\mathrm{fm}] = 0.064$

- Runs at finer lattice spacing are still ongoing.



- On large lattices, when integration of the MD eqs. is stable:

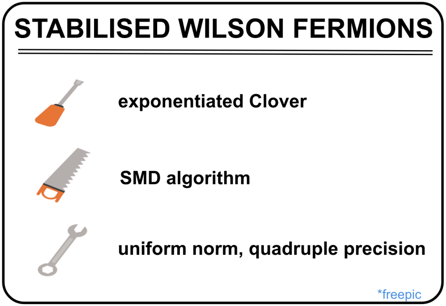
$$\rho(h) \sim \exp\left[-\frac{(\Delta H - \frac{1}{2}\sigma^2)^2}{2\sigma^2}\right], \text{ with } \sigma \text{ from } \langle P_{acc}\rangle = 1 - \frac{\sigma}{\sqrt{2\pi}} + \mathcal{O}(\sigma^3)$$

Prospects and summary

◦ Intensity frontier poses unique challenges to the lattice community.

◦ Larger volumes, finer lattice spacings need to be reached.

◦ Algorithmic developments will play an important role.



◦ We presented a toolkit to stabilise Wilson fermions, making them fit for the intensity frontier and beyond (e.g. masterfield simulations).

◦ So far we see:

- Good behaviour, also for (light,) coarse lattices.
- Measures do not introduce a significant runtime deficit.
- No indication of unusually large lattice effects.

$\rightsquigarrow$ eClover hints at an advantage.

◦ Ongoing: Further tests of continuum limit scaling behaviour.

More stable calculations in larger volumes possible.

Exciting prospects and an interesting challenge!

Thank you for your attention.